

## A Computer Simulation of the Recombination Process at Semiconductor Surfaces

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A rigorous computer simulation of the surface recombination process is made. It is shown that the surface recombination velocity,  $S$ , is not a characteristic constant of the surface as is usually assumed, but is a complicated function of charge neutrality level of surface states, sign and amount of fixed charge, substrate doping level and profile, and light intensity and spectrum. It is also shown that  $S$  can be reduced by introducing a suitable amount of a fixed charge or by forming a highly doped surface layer. Effect of device doping profile on  $S$  is also discussed.

### 1. INTRODUCTION

Recombination processes through surface states play important roles in semiconductor devices such as solar cells, bipolar transistors and opto-electronic devices. Recent device trends of utilizing thin layered structures and reducing feature sizes, as are evident, for example, in thin-substrate Si high efficiency solar cells and GaAs/AlGaAs HBTs with reduced emitter sizes, make the role of the surface more and more important with respect to the bulk.

Surface recombination is usually described by the surface recombination velocity,  $S$ , a single parameter which is assumed to be a characteristic constant of a given surface.

In the present paper, a computer program has been developed for a rigorous simulation of the surface recombination process. The result of simulation shows that the surface recombination velocity  $S$  is not a characteristic constant of the surface, but depends strongly on the location of the charge

neutrality level of surface states, sign and amount of fixed charge, doping level and profile, and light intensity and spectrum. It is also shown that  $S$  can be reduced by introducing a fixed charge or by forming a highly doped surface layer.

### 2. METHOD OF SIMULATION

For simulation, a U shaped surface state continuum schematically shown in Fig.1(a), is assumed, based on the the unified disorder induced gap state (DIGS) model<sup>1,2</sup>) The continuum consists of donor (bonding) and acceptor (anti-bonding) type states whose boundary is given by a characteristic charge neutrality level,  $E_{HO}$ , where the state density becomes minimum.  $E_{HO}$  lies at  $E_C - 0.7$  eV for Si,  $E_C - 0.9$  eV for GaAs and  $E_C - 0.35$  eV for InP, respectively. The following mathematical expression for the donor and acceptor states was used.

$$N_{SS} = N_{SS0} \exp \left\{ \frac{(E - E_{HO})}{E_0} \right\}^n \quad (1)$$

The physical situation under consideration is schematically shown in Fig.1 (b) for a n-type semiconductor under illumination. An overall self-consistency should be established among recombination, generation, carrier flows, various charge contributions, band-bending, DIGS occupation and quasi-Fermi levels. To rigorously deal with such a complicated situation, a one-dimensional Scharfetter-Gummel <sup>3)</sup> type vector-matrix simulation program has been developed.

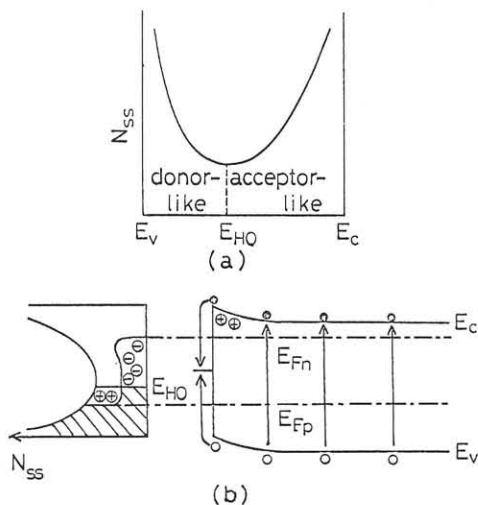


Fig.1 (a)  $N_{ss}$  distribution (b) the physical situation under illumination.

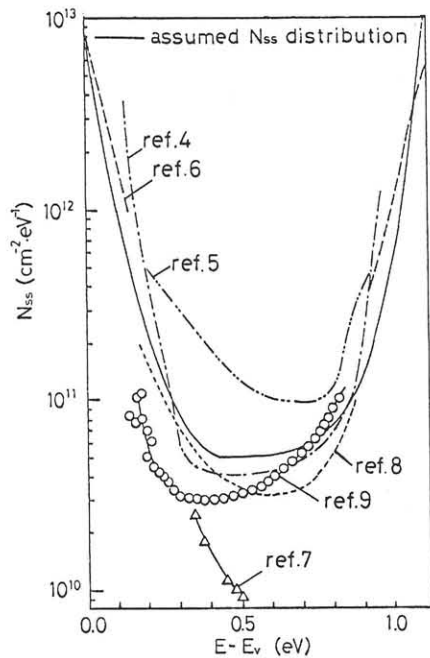


Fig.2  $N_{ss}$  distribution at Si/SiO<sub>2</sub> interface used in the simulation.

For simulation of recombination process at the Si/SiO<sub>2</sub> interface, Eq.(1) was fitted to the measured distributions reported in the literature <sup>4-9)</sup> as shown in Fig.2.

### 3.RESULTS AND DISCUSSION

#### 3.1 Surface Recombination Velocity

In order to clarify the properties of the surface recombination velocity,  $S$ , an analysis of recombination was carried out for hypothetical uniform distributions of surface states with different position of the charge neutrality level  $E_{HO}$ . Two kinds of definition of the surface recombination velocity was compared, i.e., the intrinsic surface recombination velocity,  $S_i$ , defined as the recombination rate,  $U$ , divided by the excess minority carrier concentration at the surface and the effective surface recombination velocity,  $S_{eff}$ , defined as  $U$  divided by the excess minority carrier concentration at the surface depletion /accumulation layer edge. The simulation indicated that  $S_{eff}$  is more suitable parameter to describe the surface recombination process. The calculated value of  $S_{eff}$  is plotted against the incident photon flux density in Fig.3. As seen in Fig.3,  $S_{eff}$  depends strongly on the position of  $E_{HO}$  and the incident photon flux density. It was also found that  $S_{eff}$  depends on the conduction type and doping level of the semiconductor. Thus, the usual assumption of  $S$  being a characteristic constant of the surface is not justified.

#### 3.2 $S_{eff}$ at Si/SiO<sub>2</sub> Interface and Effect of Fixed Charge

Figure 4 shows the calculated effective recombination velocity  $S_{eff}$  for an n-type Si-SiO<sub>2</sub> interface for different values of positive interface fixed charge density,  $Q_{fc}$ , and the bulk donor doping,  $N_D$ . It is seen that  $S_{eff}$  is greatly reduced by positive fixed charge. This is because the re-

sultant band-bending acts as a barrier against holes. The effect of the positive and negative charge on  $S_{eff}$  of an n-type Si-SiO<sub>2</sub> interface is shown in Fig.5. It is seen that negative fixed interface charge can also reduce  $S_{eff}$  due to formation of a barrier against electrons. The results in Figs.4 and 5 may be useful for efficiency

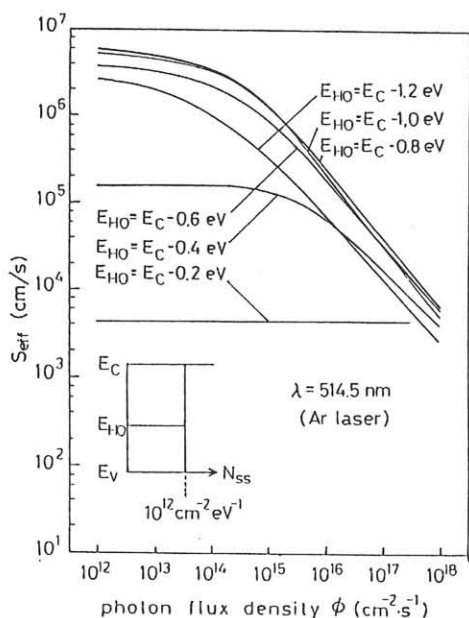


Fig.3 Effective surface recombination velocity vs. photon flux density.

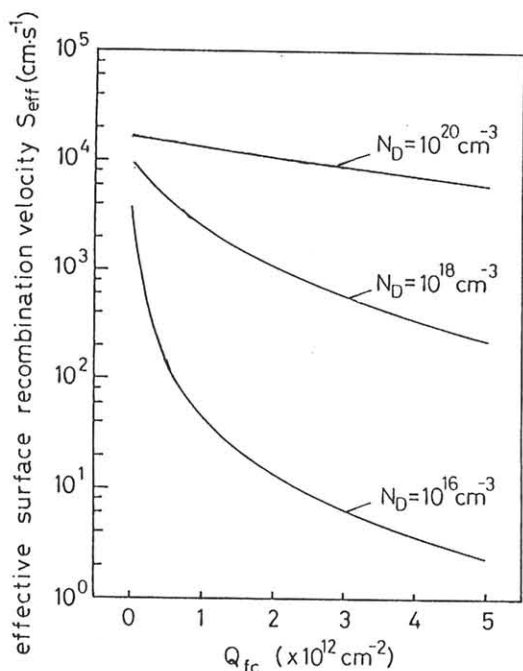


Fig.4  $S_{eff}$  vs. positive fixed charge density  $Q_{fc}$

enhancement of solar cells and recombination reduction in bipolar devices. The implication of this effect on the surface treatment techniques of compound semiconductors such as photochemical oxidation and sulfur deposition was discussed elsewhere. 10,11).

It is also noted that the values of  $S_{eff}$  in Figs. 4 and 5 are much higher than the often cited of values of 1-10 cm/s for the Si MOS system<sup>12)</sup>. This is because that the latter values are obtained by the MOS capacitance transient method where the generation rate only through mid-gap states is measured. On the other hand, under photo-excitation or carrier injection as in solar cells, bipolar transistors or opto-electronic devices, a wide range of states in the continuum take part in the recombination process, resulting in a larger  $S_{eff}$ .

### 3.3 Effect of Doping Profile

Devices such as solar cells and bipolar transistors possess complicated doping profiles, whereas the standard measurement method of the surface recombination velocity by photodecay in time domain<sup>13)</sup> or in fre-

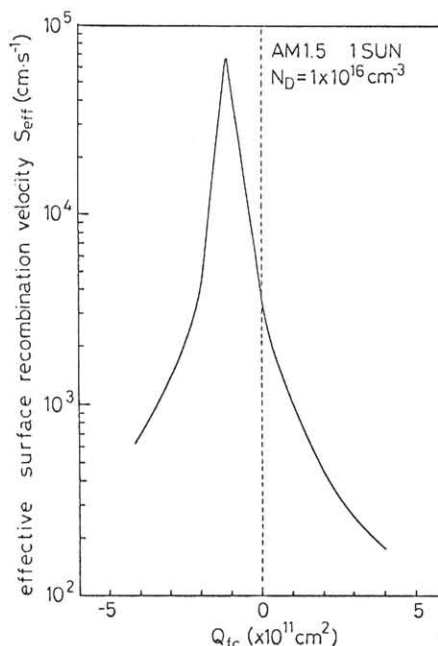


Fig.5  $S_{eff}$  of Si-SiO<sub>2</sub> interface vs. positive and negative fixed charge.

quency domain<sup>14)</sup> assumes a uniformly doped semiconductor slab for the data analysis. In order to clarify the effect of the doping profile on the effective surface recombination velocity, a detailed simulation has been made. An example of the result is shown in Fig.6 for  $n^+/n$  structure. Here,  $S_s$  and  $S_n$  are the effective surface recombination velocities evaluated at the surface and at the depletion layer edge of the n-type substrate, respectively. It is seen that  $S_n$  is much smaller than  $S_s$ . A similar result has also been obtained for an  $n^+/p$  structure. The dashed line in Fig.6 is the calculated value of  $S_n$  using the simple formula given in the figure, which agrees with simulation.

The implication of the above result is twofold. Firstly, in the design or simulation of devices such as solar cells, the value of the surface recombination velocity to be used as the surface boundary condition is  $S_s$ , whereas the standard measurement gives the value of  $S_n$  or some other value depending on the measurement set-up. Thus, a suitable conversion from the measured value to the surface value must be made. Second-

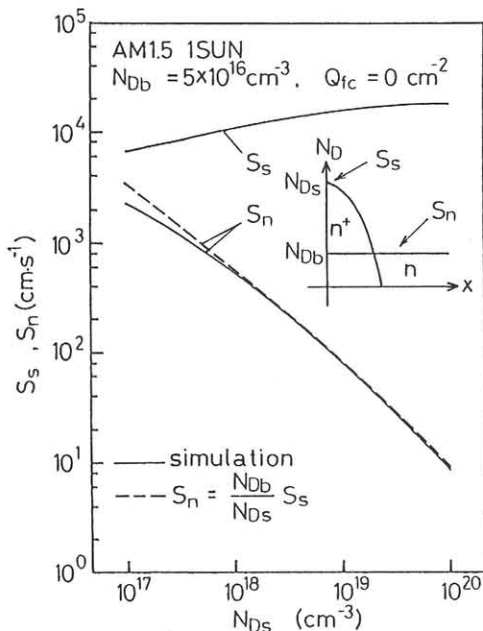


Fig.6 Effective surface recombination velocities at surface( $S_s$ ) and in bulk( $S_n$ ) of a  $\text{SiO}_2/n^+-\text{Si}/n-\text{Si}$ .

ly, when surface recombination in a semiconductor slab should be reduced, formation of a highly doped layer of the same or opposite conduction type is an effective mean.

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